# Chemistry in CFAST

Parameters which are important:

HCR - hydrogen to carbon ratio in the fuel O2 - oxygen in the fuel
OD - soot (assumed carbon) in kg per kg of $CO_2$ produced
HCN and HCL - detracts from the fuel
CO - kg of carbon monoxide per kg of carbon dioxide produced
TUHC is what is left over!

It is important to realize that the model does not check for consistency of the chemistry. Please see the document Limits on Chemistry for guidance. The heat of combustion builds in chemical kinetics which we do not calculate *apriori*. Energy release is calculated from the amount of fuel consumed, which is constrained by the oxygen available at the point of combustion. Given the rate of oxygen consumption, oxygen calorimetry yields the heat release rate. The HRR for this process is 13.7 MJ/kg of oxygen.

The default we use for calibration, that is the default for deriving energy and mass balance, is methane. It has a heat of combustion of approximately 50 MJ/ kg, which includes breaking four hydrogen-carbon bonds, and their concomitant combining with oxygen.

There are several aspects of chemistry which are NOT incorporated, for example we do not worry about OH radicals. Nor do we worry about $H_2$. Another assumption is that the mass of soot is carbon. As far as mass balance is concerned, this is reasonable, but there could be anomalous energy bound in the hydrogen.

The hydrogen-carbon ratio is the ratio of hydrogen in the fuel to carbon in the fuel. We have tested this up to 1/3, which is the ratio for methane. The lower limit is zero, and we have tested it (essentially) to this level, using a (mostly) carbon as a test fuel. We have not done this in a full scale test, so one might say it is unverified. But the answer is as close as we can hope for laboratory scale experiments.

As far as energy balance is concerned, higher values should work as well, though the issue mentioned above might become important. But we have only tested (verified) energy balance through methane.

Since the HCR ratio together with the heat of combustion implicitly includes the mass composition and chemical kinetics, it is important to get these numbers be correct for the fuel of interest. Next on the list of things to examine closely would be assumptions related to oxygen content of the fuel and whether you are looking at vitiation effects. The oxygen content is not too important except that it affects the fuel efficiency and does change the (effective) lower oxygen limit. Finally there are the $CO/CO_2$ ratio, and soot in kg/kg of $CO_2$. Given the mass that can result in carbon compounds, these two then determine where the carbon goes.

Since the branching rations (yields) affect the fuel consumption and species production, it is important to make sure all of the input is consistent, so as to produce consistent output.